Lecture 7b: Regularization

Pavlos Protopapas
Institute for Applied Computational Science
Harvard

Outline

Regularization of NN

- Norm Penalties
- Early Stopping
- Data Augmentation
- Sparse Representation
- Bagging
- Dropout

Outline

Regularization of NN

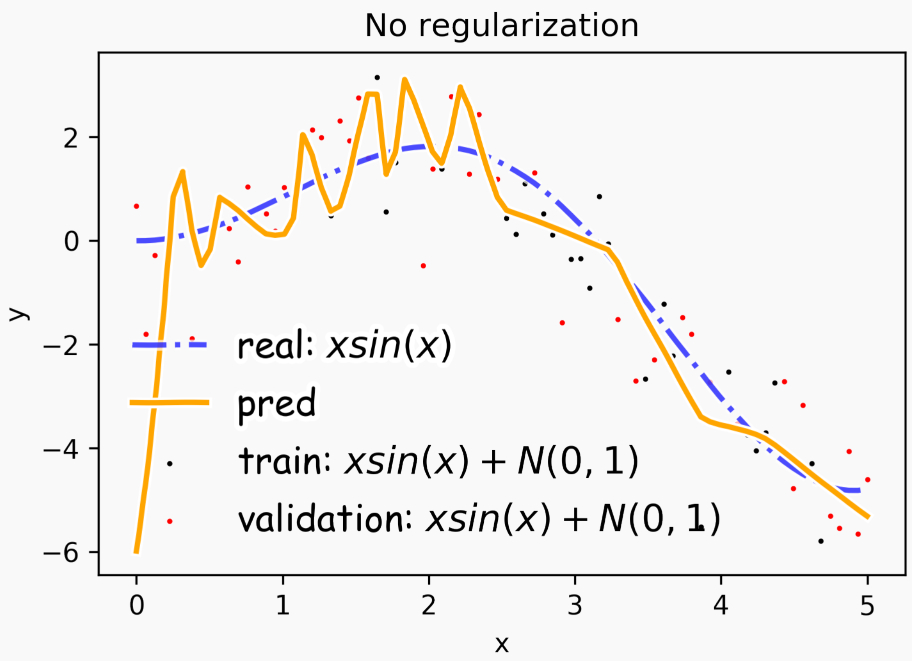
- **Norm Penalties**
- Early Stopping
- Data Augmentation
- Sparse Representation
- Bagging
- Dropout

Regularization

Regularization is any modification we make to a learning algorithm that is intended to **reduce its generalization** error but not its training error.

Overfitting

Fitting a deep neural network with 5 layers and 100 neurons per layer can lead to a very good prediction on the training set but poor prediction on validations set.



Norm Penalties

We used to optimize:

$$J(W; X, y)$$

Change to …

$$J_R(W; X, y) = J(W; X, y) + \alpha\Omega(W)$$

Biases not penalized

L_2 regularization:

- Weights decay
- MAP estimation with Gaussian prior

L_1 regularization:

- encourages sparsity
- MAP estimation with Laplacian prior

$$\Omega(W) = \frac{1}{2} \| W \|_2^2$$

$$\Omega(W) = \frac{1}{2} \| W \|_1$$

Norm Penalties

We used to optimize:

Change to …

$$W^{(i+1)} = W^{(i)} - \lambda \frac{\partial J}{\partial W}$$

$$J_R(W; X, y) = J(W; X, y) + \frac{1}{2} \alpha W^2$$

$$W^{(i+1)} = W^{(i)} - \lambda \frac{\partial J}{\partial W} \boxed{- \lambda \alpha W}$$

weights decay in proportion to its size.

Biases not penalized

L_2 regularization:

- **Decay of weights**
- MAP estimation with Gaussian prior

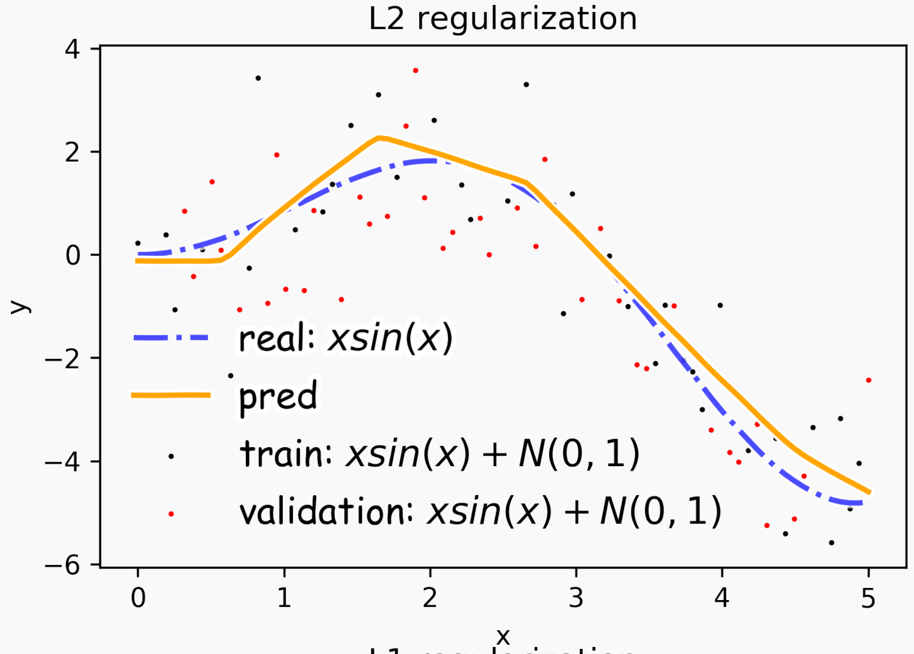
L_1 regularization:

- encourages sparsity
- MAP estimation with Laplacian prior

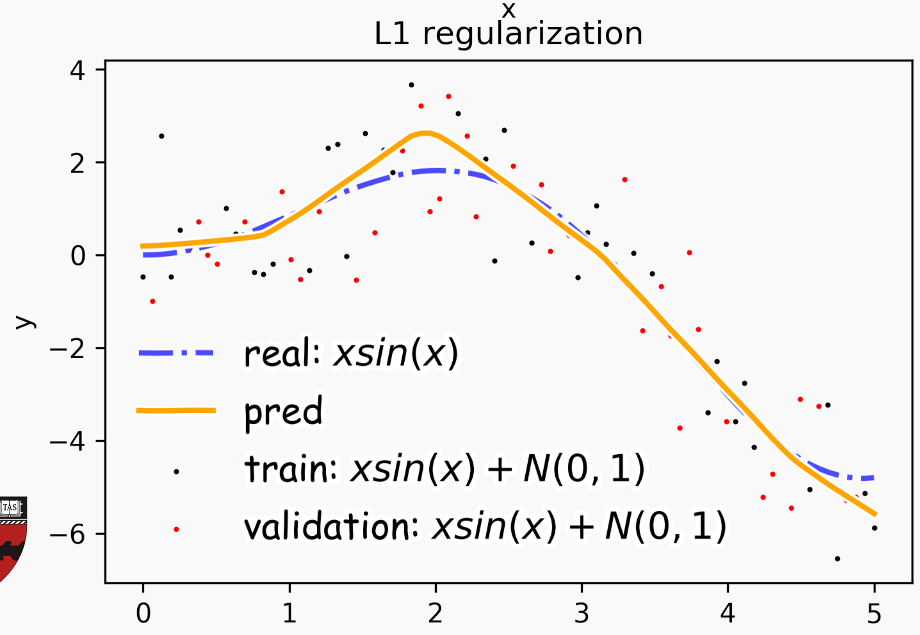
$$\Omega(W) = \frac{1}{2} \parallel W \parallel_2^2$$

$$\Omega(W) = \frac{1}{2} \parallel W \parallel_1$$

Norm Penalties



$$\Omega(W) = \frac{1}{2} \parallel W \parallel_2^2$$



$$\Omega(W) = \frac{1}{2} \parallel W \parallel_1$$

Norm Penalties as Constraints

$$\min_{\Omega(W)\leq K} J(W;X,y)$$

Useful if K is known in advance

Optimization:

- Construct Lagrangian and apply gradient descent
- Projected gradient descent

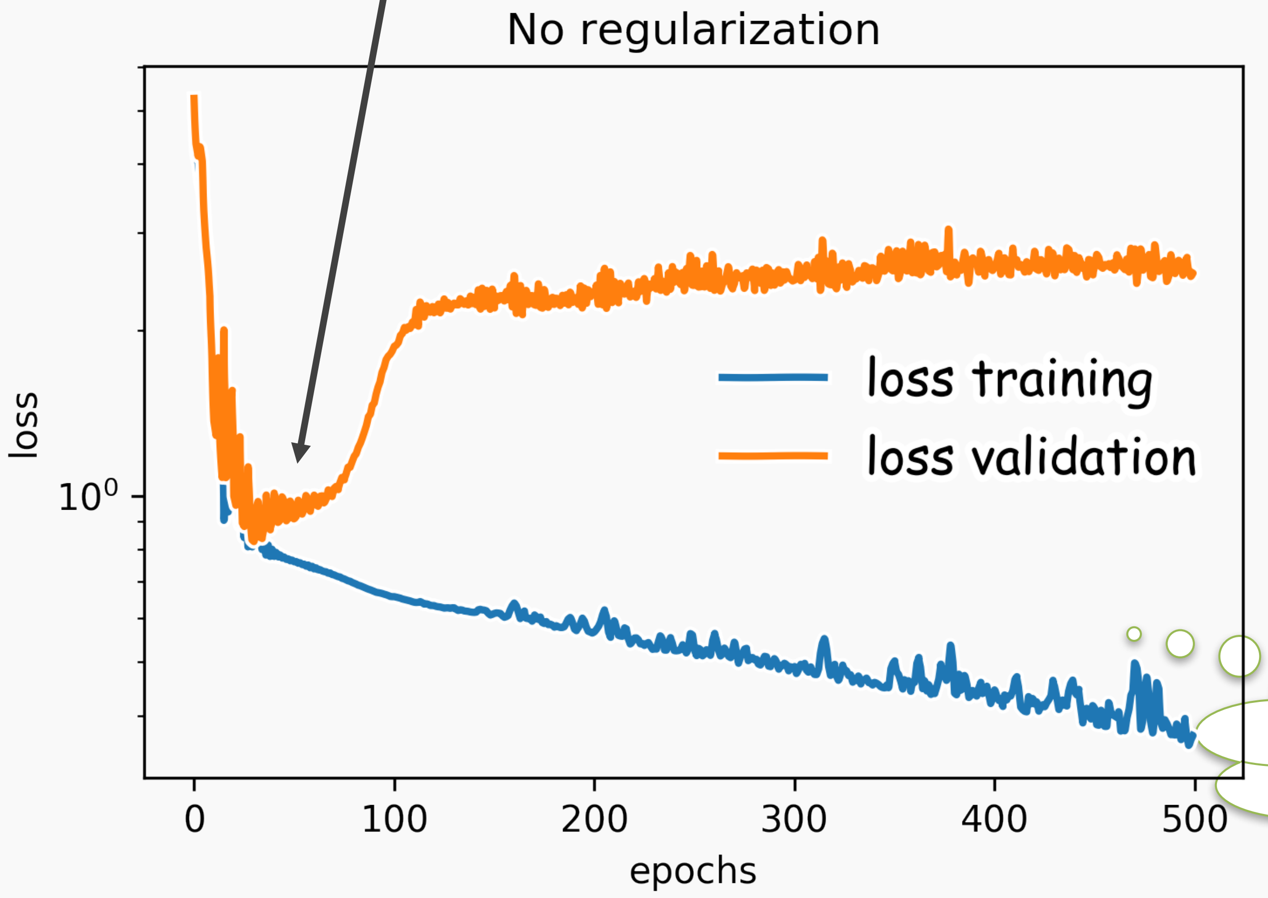
Outline

Regularization of NN

- Norm Penalties
- **Early Stopping**
- Data Augmentation
- Sparse Representation
- Bagging
- Dropout

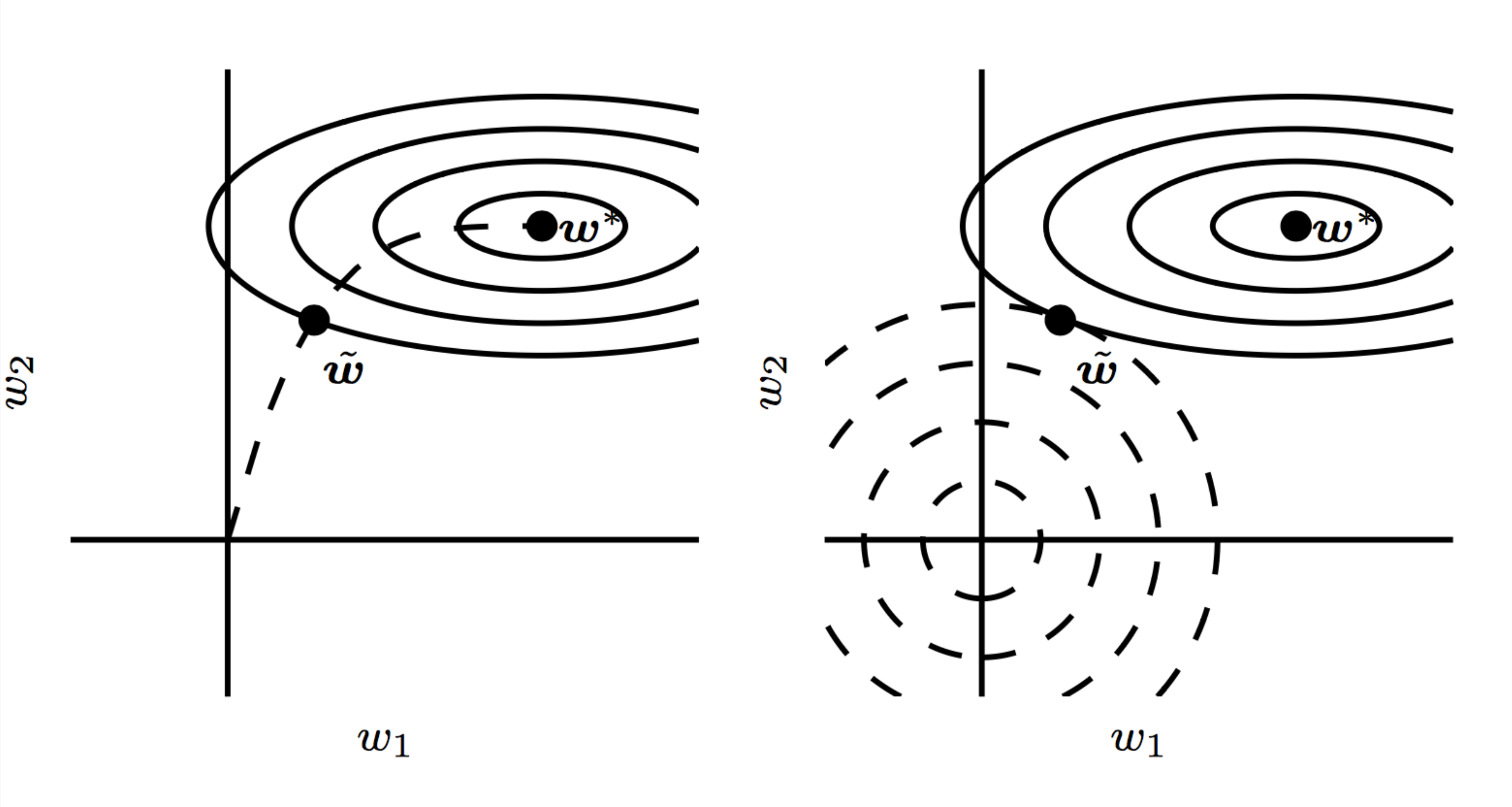
Early Stopping

Early stopping: terminate while validation set performance is better



Training time can be treated as a hyperparameter

Early Stopping

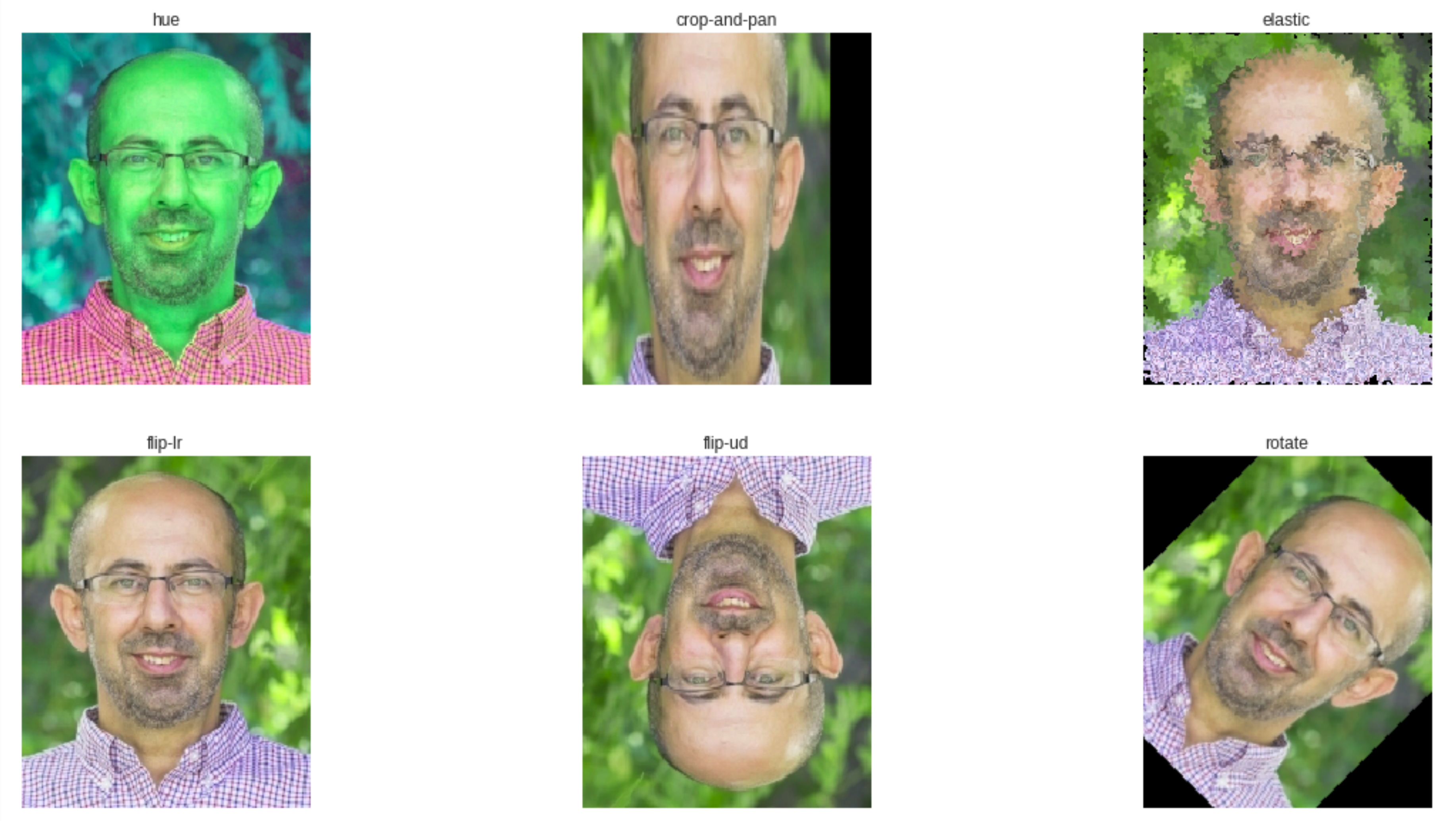


Outline

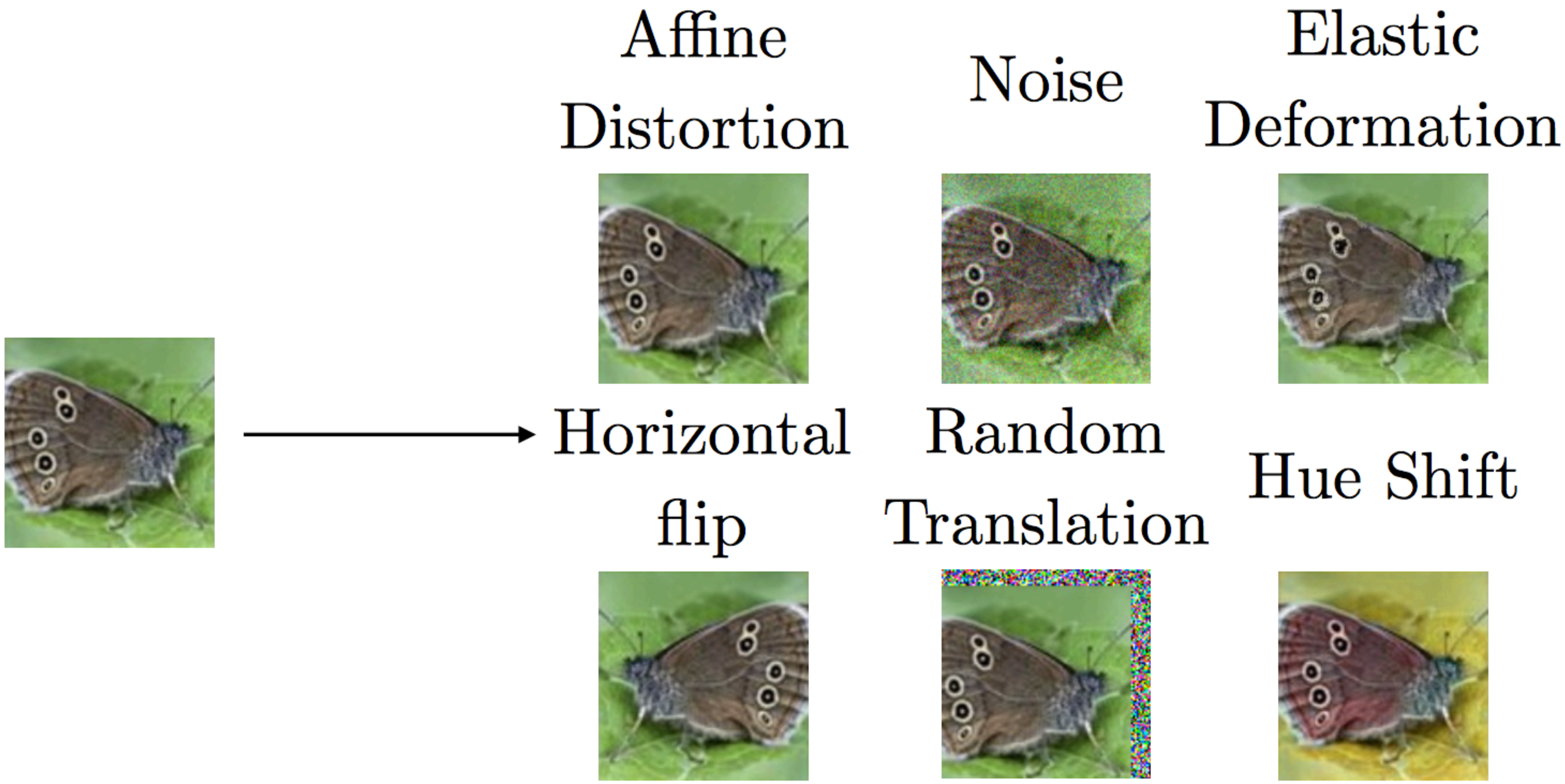
Regularization of NN

- Norm Penalties
- Early Stopping
- **Data Augmentation**
- Sparse Representation
- Bagging
- Dropout

Data Augmentation



Data Augmentation

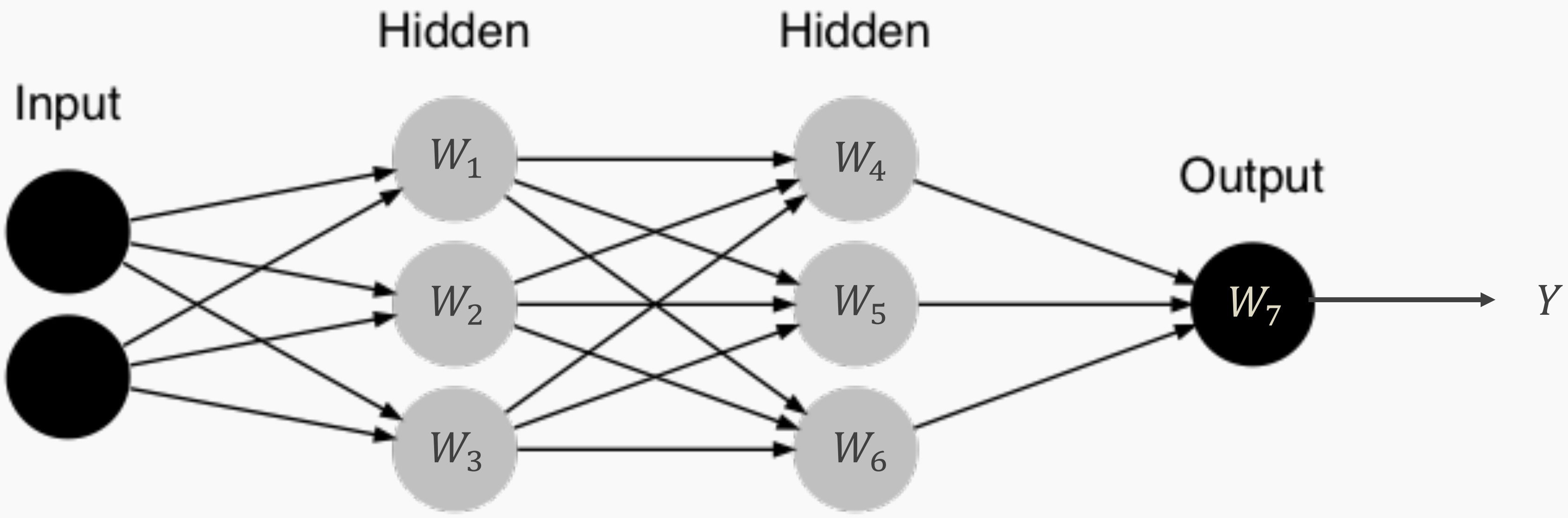


Outline

Regularization of NN

- Norm Penalties
- Early Stopping
- Data Augmentation
- **Sparse Representation**
- Bagging
- Dropout

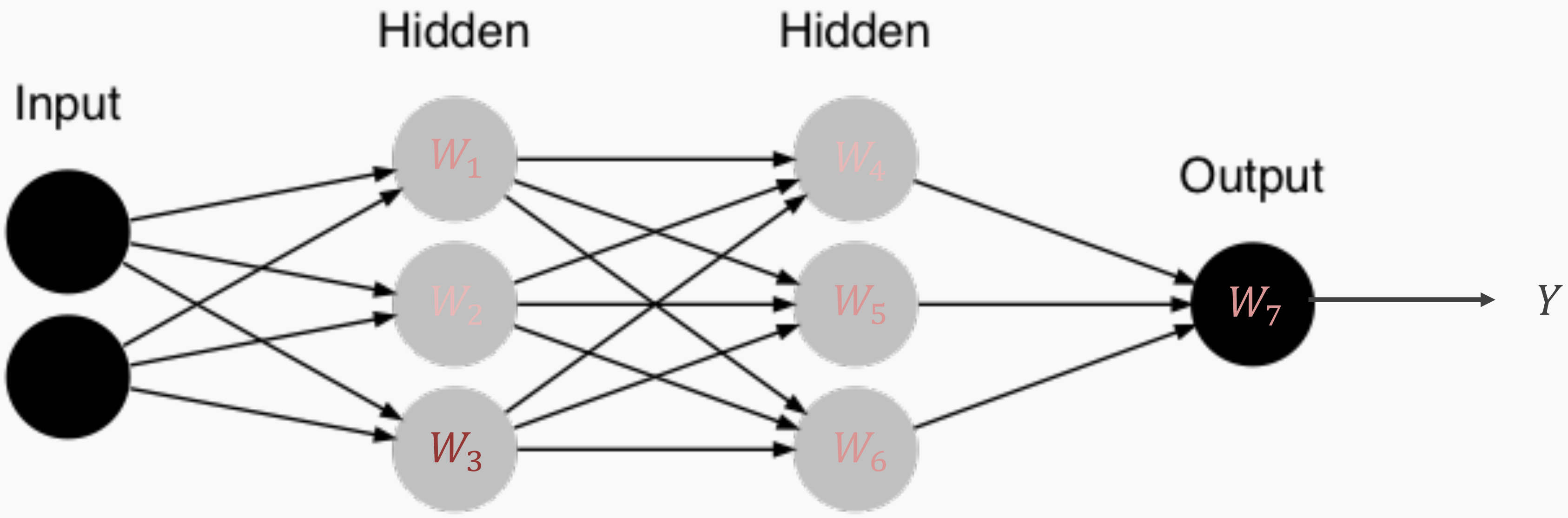
Sparse Representation



$$J(\theta; X, y)$$

$$[4.34] = \underbrace{[3.2 \quad 2.0 \quad 1.8]}_{W_7} \begin{bmatrix} 2 \\ -2.2 \\ 1.3 \end{bmatrix}$$

Sparse Representation

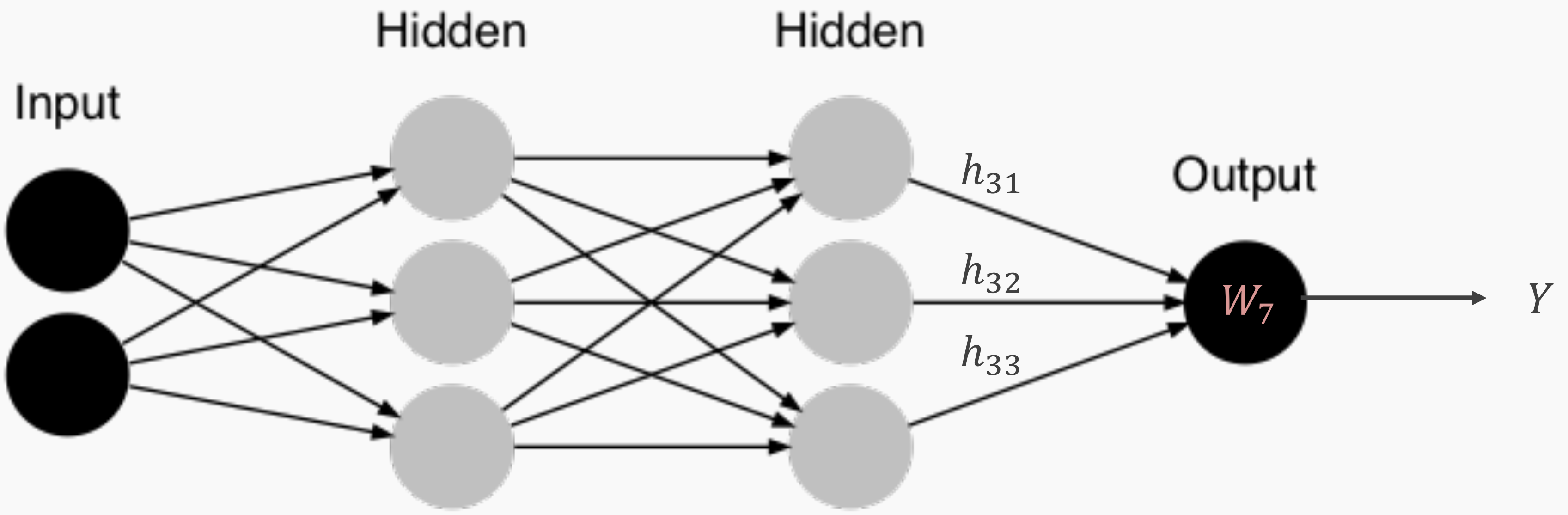


$$J_R(W;X,y) = J(\theta;X,y) + \alpha\Omega(W)$$

$$[0.69] = \underbrace{[0.5 \quad .2 \quad 0.1]}_{W_7} \begin{bmatrix} 2 \\ -2.2 \\ 1.3 \end{bmatrix}$$

Weights in output layer

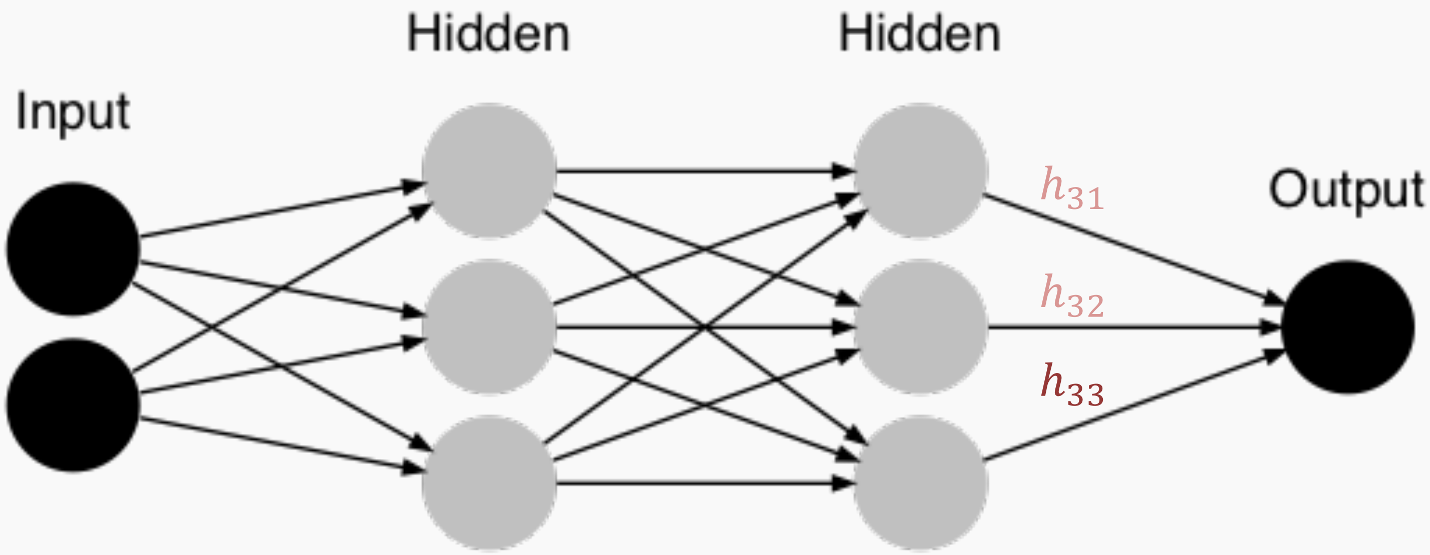
Sparse Representation



$$J(\theta; X, y)$$

$$[4.34] = [3.2 \quad 2 \quad 1] \left.\begin{bmatrix} 2 \\ -2.2 \\ 1.3 \end{bmatrix}\right\} h_{31}, h_{32}, h_{33}$$

Sparse Representation



$$J_R(W;X,y) = J(\theta;X,y) + \alpha\Omega(h)$$

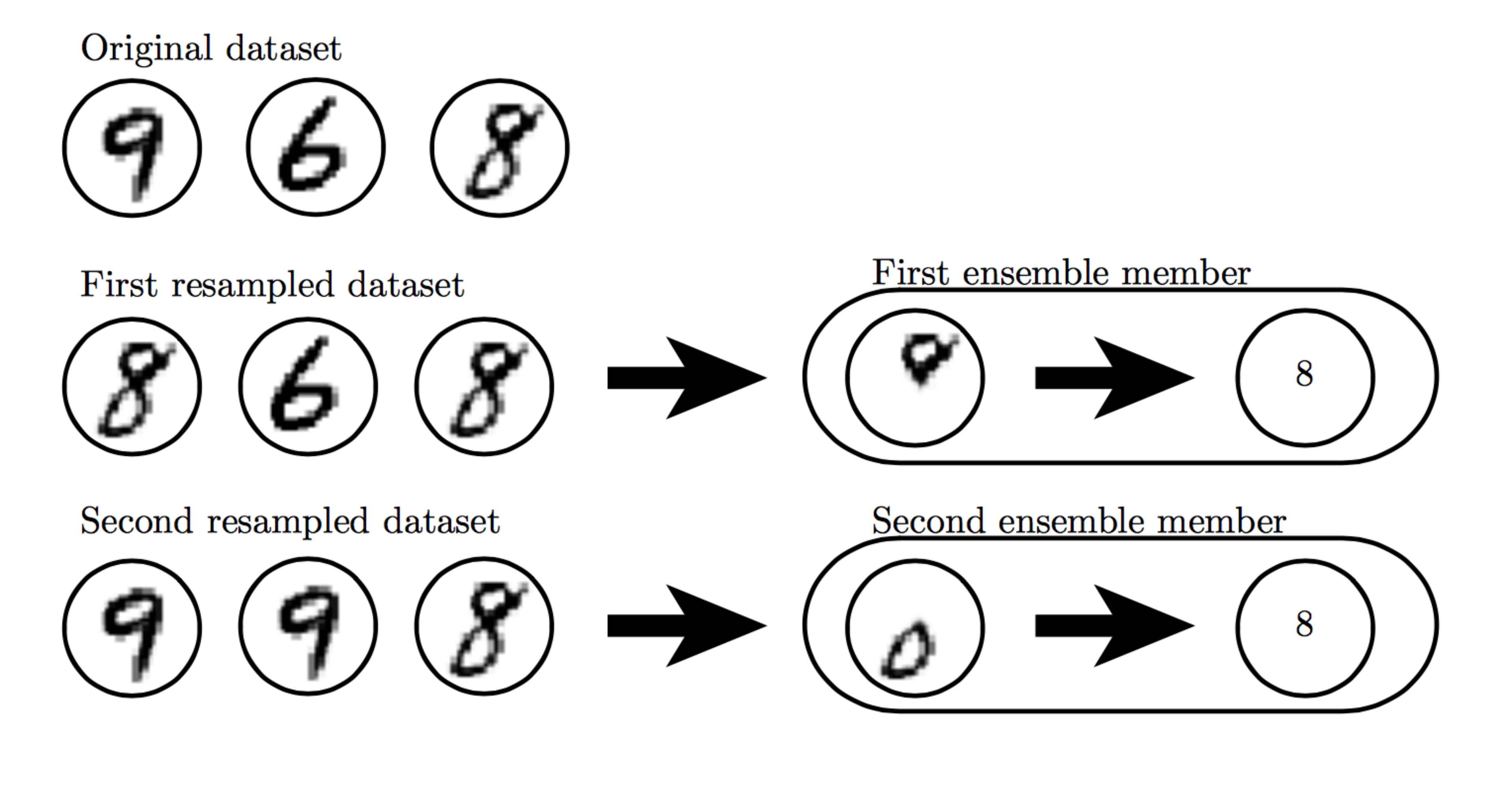
$$[1.3] = [3.2 \quad 2 \quad 1]\left.\begin{bmatrix}0\\-0.2\\.9\end{bmatrix}\right\} h_{31}, h_{32}, h_{33}$$

Output of hidden layer

Outline

Regularization of NN

- Norm Penalties
- Early Stopping
- Data Augmentation
- Sparse Representation
- **Bagging**
- Dropout


Original dataset
First resampled dataset
First ensemble member
8
Second resampled dataset
Second ensemble member
8

Outline

Regularization of NN

- Norm Penalties
- Early Stopping
- Data Augmentation
- Sparse Representation
- Bagging
- **Dropout**

Noise Robustness

Random perturbation of network weights

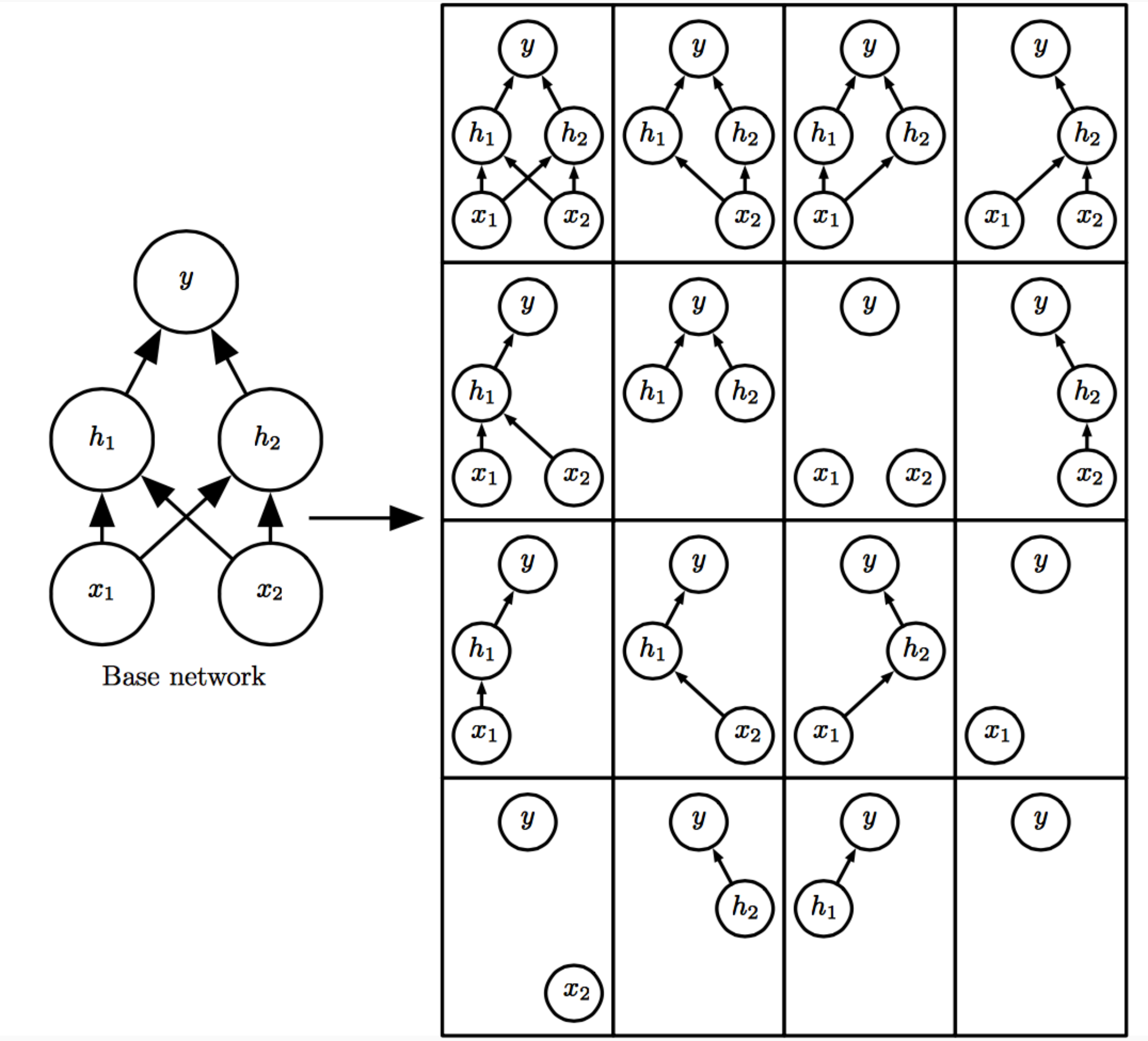
- Gaussian noise: Equivalent to minimizing loss with regularization term
- Encourages smooth function: small perturbation in weights leads to small changes in output

Injecting noise in output labels

- Better convergence: prevents pursuit of hard probabilities

Dropout

Train all sub-networks obtained by removing non-output units from base network



Ensemble of subnetworks

Dropout: Stochastic GD

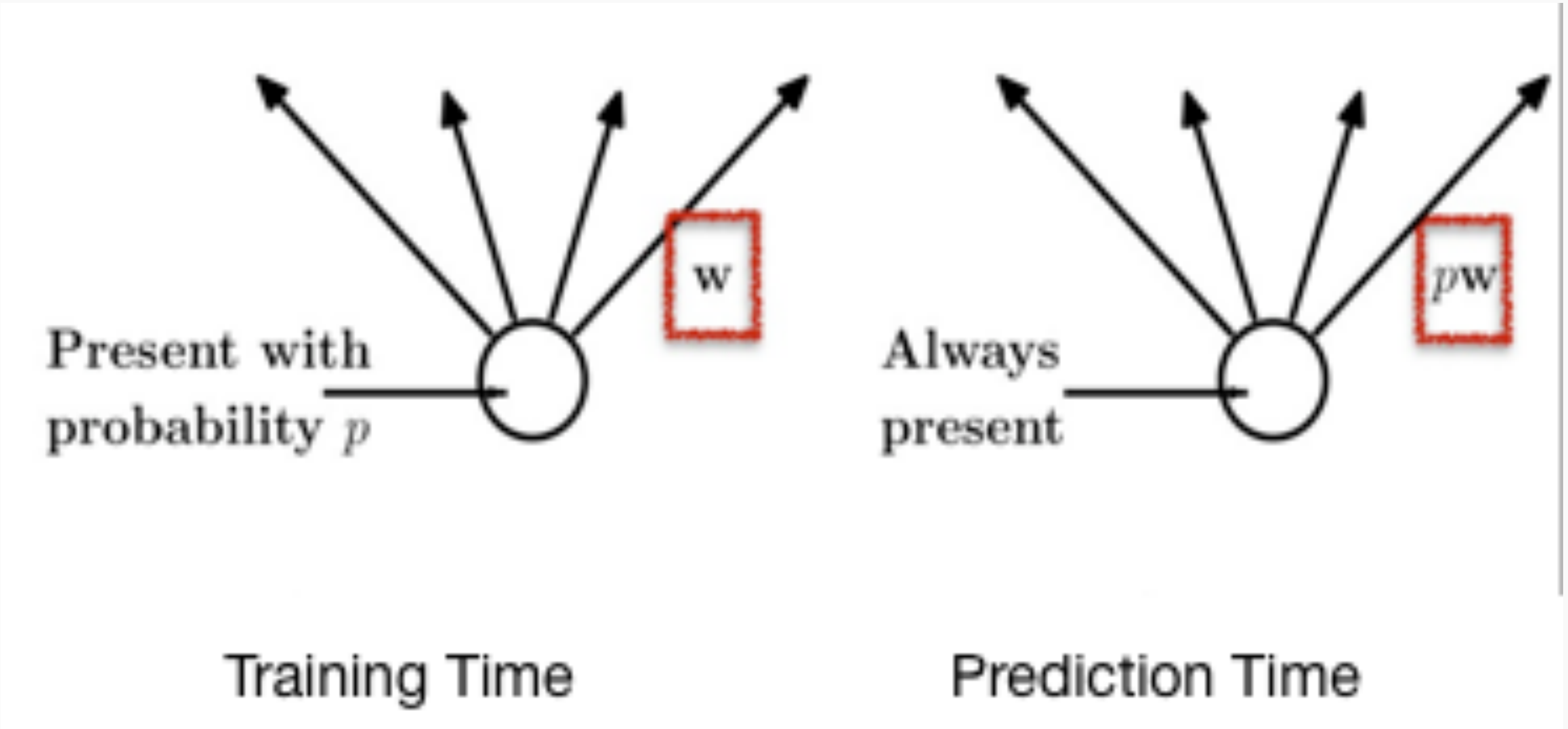
For each new example/mini-batch:

- Randomly sample a binary mask μ independently, where μ_i indicates if input/hidden node i is included
- Multiply output of node i with μ_i, and perform gradient update

Typically, an input node is **included** with **prob=0.8**, hidden node with **prob=0.5.**

Dropout: Weight Scaling

During prediction time use all units, but scale weights with probability of inclusion

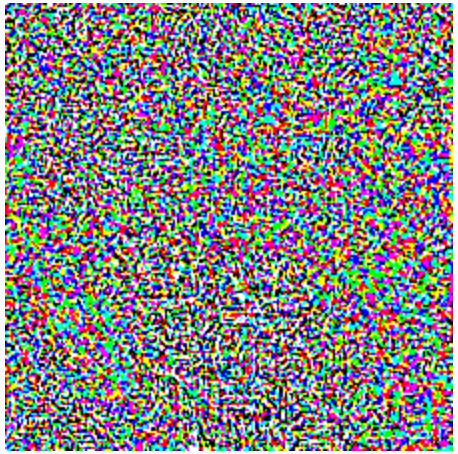


Adversarial Examples

Adversarial Examples

Panda 57% confidence

+



noise

=

Gibbon 99.3% confidence

Training on adversarial examples is mostly intended to improve security, but can sometimes provide generic regularization.

Recap

Regularization of NN

- Norm Penalties
- Early Stopping
- Data Augmentation
- Sparse Representation
- Bagging
- Dropout